Phase transitions in a one-dimensional multibarrier potential of finite range

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Abstract

We have previously studied properties of a one-dimensional potential with N equally spaced identical barries in a (fixed) finite interval for both finite and infinite N. It was observed that scattering and spectral properties depend sensitively on the ratio c of spacing to width of the barriers (even in the limit $N \to \infty$). We compute here the specific heat of an ensemble of such systems and show that there is critical dependence on this parameter, as well as on the temperature, strongly suggestive of phase transitions.

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I. INTRODUCTION

We have studied the one-dimensional locally periodic multibarrier potential of finite range for both finite and infinite number N of barriers. We found [1] that there is a critical dependence of the transmission coefficient, the cross section and the distribution of poles of the S-matrix [2] on the ratio c of the total interval between the barriers to their total width. Under certain conditions this model was found to contain signatures of chaotic behaviour [3].

We discuss in this work thermodynamic properties [4] such as the specific heat and the entropy of an ensemble of such systems and show that they also depend critically upon this ratio in addition to their dependence upon the temperature. We show that when the number of barriers is not large there are no low-lying energy eigenvalues for small values of the ratio c. These values of c depend upon the value of the number N of barriers in such a manner that the ranges of c in which this part of the energy spectrum is missing increase at first with N and then decrease as N continue to grow until they disappear entirely for large enough N. Above the upper boundaries of these ranges are the points where the energy spectrum contains eigenvalue distribution over all energies. This apparently accounts, even for neighbouring values of c within these ranges, for large changes in the average energy and all the other statistical mechanics properties, such as specific heat and entropy, derived from it. For example, the corresponding curves of the specific heat, for these neighbouring values of c, as functions of the temperature, differ markedly from each other, as will be shown in the following, when plotting these curves in a single figure. This sensitivity of the specific heat is largest for intermediate values of N and c in which the curves of the specific heats as functions of the temperature differ to the extent that some of them exhibit double peak phase transitions while other curves, for neighbouring values of c, resemble the conventional Debye curve [4] which characterizes the solid crystal. For infinite N, as will be shown, the double peak phase phenomenon is retained even for large values of c. Also, we find, for all values of N and c, indication of phase transitions at small values of the temperature T. We note that for any c, which is greater than some value which depends upon N, the system behaves for all N, except for a spike form at small T, in a manner similar to that of the solid crystals in which the constituent atoms are widely separated, and thus, as we have remarked, are characterized by large values of the ratio c. This is seen on the corresponding graphs of the specific heats as functions of the temperature which have the same form as that of Debye.

In Section 1 we study the properties of a one-dimensional N potential barrier system when N is a finite number. In Section 2 we study the limit of $N \to \infty$ (in the same fixed interval). For both cases we find abrupt and large changes in the values of specific heat and entropy for small values of the temperature T. These large changes suggest the existence of phase transitions. In particular, for intermediate N and c, we find double peaks [5–8] in the specific heat curves. Double peak phase transitions appear, especially, for infinite N in which it remains effective even for large values of c. Tanaka et al [6] have found double peak structures in anti-ferromagnetic materials, corresponding to magnetic phases, where the external magnetic field seems to play a role somewhat analogous to the parameter c in our study. Leung and Neda [5] and also Kim et al [7] have found double peaks in the response curves, apparently associated with dynamically induced phase transitions. Ko and

Asakawa [8] have also found a double peak structure in their calculations of the phases of a quark-gluon plasma, where one may think of a large number of interactions in a bounded region.

II. THE ONE-DIMENSIONAL N POTENTIAL BARRIER SYSTEM

We consider a finite N barrier system where all these barriers have the same height v and are locally periodic in the finite interval. This array is assumed to start at the point $x = -\frac{a+b}{2}$ and ends at $x = \frac{a+b}{2}$, so that the total length of this system is $L = a + b$. Here a is the total width of all the N barriers (where $v \neq 0$), and b is the total sum of all the intervals between neighbouring barriers (where $v = 0$). Thus, since we have N potential barriers the width of each one is $\frac{a}{N}$, and the interval between each two neighbouring ones is $\frac{b}{N-1}$. Denoting $b = ac$ where c is a real number we can express a and b in terms of L and c as

$$a = \frac{L}{1+c}, \qquad b = \frac{Lc}{1+c} \tag{1}$$

Let us first consider the passage of a plane wave through this system, which has the form $\phi = Ae^{ikx}$, $-\frac{a+b}{2} \leq x \leq \frac{a+b}{2}$. Matching boundary conditions at the beginning and end of each barrier, we may construct a solution in terms of the transfer matrices [2,10] $P^{(j)}$ on the jth barrier. After the nth barrier we obtain, using the terminology in [2]

$$\begin{bmatrix} A_{2n+1} \\ B_{2n+1} \end{bmatrix} = P^{(n)} P^{(n-1)} \dots P^{(2)} P^{(1)} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} \tag{2}$$

A_{2n+1} and B_{2n+1} are the amplitudes of the transmitted and reflected parts respectively of the wave function at the nth potential barrier. A_0 is the coefficient of the initial wave that approaches the potential barrier system, and B_0 is the coefficient of the reflected wave from the first barrier. $P^{(n)}$ is the product of three two dimensional matrices

$$P^{(n)} = M_n T \grave{M}_n = \tag{3}$$
$$= \begin{bmatrix} e^{-ik(\frac{(n-1)b}{N-1}+\frac{(2n-1)a}{2N})} & 0 \\ 0 & e^{ik(\frac{(n-1)b}{N-1}+\frac{(2n-1)a}{2N})} \end{bmatrix} \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} e^{ik(\frac{(n-1)b}{N-1}+\frac{(2n-3)a}{2N})} & 0 \\ 0 & e^{-ik(\frac{(n-1)b}{N-1}+\frac{(2n-3)a}{2N})} \end{bmatrix}$$

The middle matrix T does not depend on n and its components are given by

$$T_{11} = \cos(\frac{aq}{N}) + i\frac{\xi}{2}\sin(\frac{aq}{N}), \quad T_{12} = i\frac{\eta}{2}\sin(\frac{aq}{N}) \tag{4}$$
$$T_{21} = -i\frac{\eta}{2}\sin(\frac{aq}{N}), \quad T_{22} = \cos(\frac{aq}{N}) - i\frac{\xi}{2}\sin(\frac{aq}{N})$$

k is $\sqrt{\frac{2me}{\hbar^2}}$, q is $\sqrt{\frac{2m(e-v)}{\hbar^2}}$ (in the numerical part of this work we assign $\hbar = 1$, and $m = \frac{1}{2}$), and ξ and η are given by

$$\xi = \frac{q}{k} + \frac{k}{q}, \quad \eta = \frac{q}{k} - \frac{k}{q} \tag{5}$$

The diagonal matrices M_n and $\grave{M}_n$ that multiply the constant identical matrices T depend on n but as can be seen from the equations (2)-(3) the product of each two neighbouring diagonal matrices $\grave{M}_n M_{n-1}$ is constant for each n. That is, $\grave{M}_n M_{n-1} = \begin{bmatrix} e^{\frac{ikb}{N-1}} & 0 \\ 0 & e^{-\frac{ikb}{N-1}} \end{bmatrix}$. Thus, using the last equations we can write Equation (2) as

$$\left[\begin{array}{c} A_{2n+1} \\ B_{2n+1} \end{array}\right] = \left[\begin{array}{cc} e^{-ik(a+b-\frac{a}{2N})} & 0 \\ 0 & e^{ik(a+b-\frac{a}{2N})} \end{array}\right] \left[\begin{array}{cc} T_{11} & T_{12} \\ T_{21} & T_{22} \end{array}\right] \left(\left[\begin{array}{cc} e^{\frac{ikb}{N-1}} & 0 \\ 0 & e^{-\frac{ikb}{N-1}} \end{array}\right] \left[\begin{array}{cc} T_{11} & T_{12} \\ T_{21} & T_{22} \end{array}\right]\right)^{n-1} \cdot$$
$$\cdot \left[\begin{array}{cc} e^{\frac{-ika}{2N}} & 0 \\ 0 & e^{\frac{ika}{2N}} \end{array}\right] \left[\begin{array}{c} A_0 \\ B_0 \end{array}\right] = Q \left[\begin{array}{c} A_0 \\ B_0 \end{array}\right] \tag{6}$$

We have denoted by Q all the two dimensional matrices that multiply the vector $\left[\begin{array}{c} A_0 \\ B_0 \end{array}\right]$.

We find, now, the energy spectrum of the dense system. We use the S-matrix and periodic boundary conditions at the two remotely placed sides of the system. That is, we assume that the wave function and its derivative at the far right end of the system, say at $x = C$ where C is much larger than the size $L = a + b$ of the system, is equal to the wave function and its derivative at the corresponding far left end of the system at $x = -C$, so we obtain $A_{2N+1}e^{ikC} = A_0 e^{-ikC}$, $B_{2N+1}e^{-ikC} = B_0 e^{ikC}$. Thus, using the last relation and the following relations between the components of the S and Q matrices [2]

$$S_{11} = Q_{11} - \frac{Q_{12}Q_{21}}{Q_{22}} = \frac{1}{Q_{22}}, \quad S_{12} = \frac{Q_{12}}{Q_{22}}, \quad S_{21} = -\frac{Q_{21}}{Q_{22}}, \quad S_{22} = \frac{1}{Q_{22}}, \tag{7}$$

we can express the dependence of the outgoing waves A_{2N+1} and B_0 upon the ingoing ones A_0 and B_{2N+1} as

$$\left[\begin{array}{c} A_{2N+1} \\ B_0 \end{array}\right] = \left[\begin{array}{cc} S_{11} & S_{12} \\ S_{21} & S_{22} \end{array}\right] \left[\begin{array}{c} A_0 \\ B_{2N+1} \end{array}\right] = e^{2ikC} \left[\begin{array}{cc} S_{11} & S_{12} \\ S_{21} & S_{22} \end{array}\right] \left[\begin{array}{c} A_{2N+1} \\ B_0 \end{array}\right] = \tag{8}$$
$$= \frac{e^{2ikC}}{Q_{22}} \left[\begin{array}{cc} 1 & Q_{12} \\ -Q_{21} & 1 \end{array}\right] \left[\begin{array}{c} A_{2N+1} \\ B_0 \end{array}\right]$$

To obtain a non trivial solution for the vector $\left[\begin{array}{c} A_{2N+1} \\ B_0 \end{array}\right]$ we have to solve the following equation

$$\det \left[\begin{array}{cc} \frac{e^{2ikC}}{Q_{22}} - 1 & \frac{e^{2ikC}Q_{12}}{Q_{22}} \\ -\frac{e^{2ikC}Q_{21}}{Q_{22}} & \frac{e^{2ikC}}{Q_{22}} - 1 \end{array}\right] = 0 \tag{9}$$

This results in the relation

$$\frac{\cos(4kC)}{Q_{22}^2} - \frac{2\cos(2kC)}{Q_{22}} + 1 + \frac{Q_{12}Q_{21}\cos(4kC)}{Q_{22}^2} + \tag{10}$$
$$+i(\frac{\sin(4kC)}{Q_{22}^2} - \frac{2\sin(2kC)}{Q_{22}} + \frac{Q_{12}Q_{21}\sin(4kC)}{Q_{22}^2}) = 0$$

The energies, satisfying this relation, depend, as noted, on c and N and are obtained numerically. We show, now, that the high energy part ($e >> v$) of the spectrum obtained from Eq (10) depends only on C and may be obtained analytically without using numerical methods. For that matter we note that when the energy e becomes very large we have $k \approx q$, and ξ and η from Eq (5) obtain the values of 2 and 0 respectively. In that case the components T_{12} and T_{21} of the two dimensional matrix T from Eq (4) become zero, and the diagonal

elements T_{11} and T_{22} become $e^{\frac{iqa}{N}}$ and $e^{-\frac{iqa}{N}}$ respectively. Thus, the two dimensional matrix Q from Eq (6) becomes much simplified and may be calculated analytically as follows (using $q \approx k$ for the very high part of the energy spectrum)

$$Q_{(high-energies)} = \begin{bmatrix} e^{-ik(a+b-\frac{a}{2N})} & 0 \\ 0 & e^{ik(a+b-\frac{a}{2N})} \end{bmatrix} \begin{bmatrix} e^{\frac{ika}{N}} & 0 \\ 0 & e^{-\frac{ika}{N}} \end{bmatrix} \left(\begin{bmatrix} e^{ik(\frac{b}{N-1}+\frac{a}{N})} & 0 \\ 0 & e^{-ik(\frac{b}{N-1}+\frac{a}{N})} \end{bmatrix} \right)^{n-1} \cdot$$

$$\cdot \begin{bmatrix} e^{-\frac{ika}{2N}} & 0 \\ 0 & e^{\frac{ika}{2N}} \end{bmatrix} = \begin{bmatrix} e^{-ik(a(1-\frac{3}{2N})+b-(n-1)(\frac{b}{N-1}+\frac{a}{N})+\frac{a}{2N})} & 0 \\ 0 & e^{ik(a(1-\frac{3}{2N})+b-(n-1)(\frac{b}{N-1}+\frac{a}{N})+\frac{a}{2N})} \end{bmatrix} =$$

$$= \begin{bmatrix} e^{-ik(a+b+\frac{b}{N=1}-n(\frac{b}{N-1}+\frac{a}{N}))} & 0 \\ 0 & e^{ik(a+b+\frac{b}{N=1}-n(\frac{b}{N-1}+\frac{a}{N}))} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{11}$$

for $n = N$, required for our application to Eq (10). Thus we see that the two dimensional matrix Q from Eq (6) becomes the two dimensional unity matrix in the limit of large energies e. Substituting the components of Q ($Q_{11} = Q_{22} = 1$, $Q_{12} = Q_{21} = 0$) in Eq (11) we obtain

$$\det \begin{bmatrix} e^{2ikC} - 1 & 0 \\ 0 & e^{2ikC} - 1 \end{bmatrix} = (e^{2ikC} - 1)^2 = 0 \tag{12}$$

The last equation is satisfied for all $k = \frac{\pi n}{C}$, $\quad n = 0, 1, 2, 3 \ldots$, but since we are restricted here to the high energy part of the energy spectrum we refer only to the large values of n.

We note that we may use the previous equations also for the $e < v$ case except that q is defined now as $\sqrt{\frac{2m(v-e)}{\hbar^2}}$. Also the components of the matrix T from Eq (4) are now

$$\begin{aligned} T_{11} &= \cosh(\frac{aq}{N}) + \frac{\grave{\xi}}{2}\sinh(\frac{aq}{N}), \quad T_{12} = \frac{\grave{\eta}}{2}\sinh(\frac{aq}{N}) \\ T_{21} &= -\frac{\grave{\eta}}{2}\sinh(\frac{aq}{N}), \quad T_{22} = \cosh(\frac{aq}{N}) - \frac{\grave{\xi}}{2}\sinh(\frac{aq}{N}), \end{aligned} \tag{13}$$

where $\grave{\xi}$ and $\grave{\eta}$ are

$$\grave{\xi} = -i\eta = \frac{q}{ik} + \frac{ik}{q}, \quad \grave{\eta} = -i\xi = \frac{q}{ik} - \frac{ik}{q}, \tag{14}$$

and η and ξ are given by Eq (5). Substituting these expressions into Eq (6) we obtain the two dimensional transfer matrix Q for the $e < v$ case. Using this Q and Eqs (7), (8) we can obtain an equation similar to Eq (10) from which we derive the energy spectrum for the $e < v$ case. Thus, the energy spectrum is composed of three parts: 1) the part for the $e < v$ case. 2) the part that satisfies $e_{n_0} > e > v$, where e_{n_0} is some arbitrarily specified large energy (these two parts are obtained numerically by solving Eq (10) for the $e > v$ case and the corresponding equation for the $e < v$ case), and 3) all the high energies that are larger than e_{n_0} and are obtained analytically using Eqs (11), (12) and the relation $k = \frac{\pi n}{C}$ $\quad n = n_0, n_0+1, n_0+2 \ldots$, where n_0 is some specified large integer that corresponds to the energy e_{n_0}. Now, since the relation between the energy e and k is $k = \sqrt{e}$ (as remarked, we assign $\hbar = 1$ and $m = \frac{1}{2}$), the high part of the energy spectrum is given by $e_{high} = (\frac{\pi n}{C})^2$, where $n = n_0, n_0 + 1, n_0 + 2, \ldots$. For the numerical part of the calculations we assign the

following values for the relevant parameters: $v = 60$, $C = 90$, $L = 20$, and $e_{n_0} = 1080$. Thus, the $e < v$ part of the spectrum is $0 < e < 60$. The second part is $60 < e < 1080$, and the third part is $e > 1080$. The n_0 that corresponds to e_{n_0} is $n_0 = \frac{C}{\pi}\sqrt{e_{n_0}} \approx 941$.

We want to obtain a formula for the average energy from which we may derive most of the statistical mechanics parameters mentioned above. This average energy depends upon c, C, N and the temperature T (the dependence upon the temperature is through $\beta = \frac{1}{\kappa T}$, where κ is the Boltzman constant which is assigned, in our numerical work, the value of unity) and is given by

$$<e>(\beta, c, N) = \frac{\sum e(c,N)e^{-\beta e(c,N)} + \sum_{941}^{\infty}(\frac{n\pi}{C})^2 e^{-\beta(\frac{\pi n}{C})^2}}{\sum e^{-\beta e(c,N)} + \sum_{941}^{\infty} e^{-\beta(\frac{\pi n}{C})^2}}, \tag{15}$$

where the first sum in the numerator and denominator is the contributions from all $e(c, N) < 1080$. For higher values of e the expressions are simpler and we take this into account in the second sum over all integers $941 \leq n$. The first sum in the numerator and denominator of Eq (15) includes the energies from the $e < v$ and the $v < e < 1080$ parts of the spectrum . These parts are obtained numerically from Eq (10) in which we substitute for the components of Q from Eq (6), using the T's of Eq (4) for the $e > v$ case, and those of Eq (13) for $e < v$. From Eq (15) we obtain an average energy for each specific triplet of values for c, N, and β, and from this average energy we may derive the quantities of statistical physics. We note that the sums over the energies from the range $0.1 \leq e \leq 1080$ depend upon the parameters N and c whereas the sums over the higher energies do not depend upon them (see Eqs (11), (12)). The specific heat C_h is obtained as the derivative of the average energy from Eq (15) with respect to the temperature T and is given by

$$\begin{aligned}
&C_h(\beta, c, N) = \frac{\partial <e>(\beta, c, N)}{\partial T} = \\
&= \frac{1}{T^2(\sum e^{-\beta e(c,N)} + \sum_{n=941}^{n=\infty} e^{-\beta(\frac{\pi n}{C})^2})^2}[\sum e^2(c,N)e^{-\beta e(c,N)} \sum e^{-\beta e(c,N)} + \\
&+ \sum e^2(c,N)e^{-\beta e(c,N)} \sum_{n=941}^{n=\infty} e^{-\beta(\frac{\pi n}{C})^2} + \sum_{n=941}^{n=\infty}(\frac{n\pi}{C})^4 e^{-\beta(\frac{\pi n}{C})^2} \sum e^{-\beta e(c,N)} + \\
&+ \sum_{n=941}^{n=\infty}(\frac{n\pi}{C})^4 e^{-\beta(\frac{\pi n}{C})^2} \sum_{n=941}^{n=\infty} e^{-\beta(\frac{\pi N}{C})^2} - (\sum e(c,N)e^{-\beta e(c,N)} \sum e(c,N)e^{-\beta e(c,N)} + \\
&+ \sum e(c,N)e^{-\beta e(c,N)} \sum_{n=941}^{n=\infty}(\frac{n\pi}{C})^2 e^{-\beta(\frac{\pi N}{C})^2} + \sum_{n=941}^{n=\infty}(\frac{n\pi}{C})^2 e^{-\beta(\frac{\pi N}{C})^2} \sum e(c,N)e^{-\beta e(c,N)} + \\
&+ \sum_{n=941}^{n=\infty}(\frac{n\pi}{C})^2 e^{-\beta(\frac{\pi n}{C})^2} \sum_{n=941}^{\infty}(\frac{n\pi}{C})^2 e^{-\beta(\frac{\pi N}{C})^2})]
\end{aligned} \tag{16}$$

It is found that for large values of the temperature T the curves of the specific heats C_h, for all values of c and N, tend to the constant value $C_h = 0.55$. That is, for these T's the curves of C_h become as expected a constant curve as for Dulong-Petit [4]. Also, for small T's the curves of C_h, for all c and N, rise rapidly to their maximum values $C_{h_{max}}$ from which they descend either to the asymptotic value of 0.55 for large T as noted or to some minimum from which they rise again to a second peak that descends to the value of 0.55 for large T. We note that the $C_{h_{max}}$'s are points that have no derivative and so they are phase transition

points [9]. The values of these $C_{h_{max}}$, however, as well as the behavior of the specific heat for intermediate values of T depend upon c and N. It has been found that for large c the curves of the specific heats, as functions of T, are of the Debye type [4], that is, the rapid approach to maximum $C_{h_{max}}$ for small T and the immediate decrease to a constant value as T grows. For small c, however, the forms of the specific heat C_h for intermediate T depart markedely from that of Debye, and the range of T in which C_h is different depends upon N in such a manner that this range increases as N grows. For example, when $N = 2$ this range is $0.4 \leq T \leq 3.8$, for $n = 35$ it is $0.4 \leq T \leq 100$ and for $N = 250$ this range increases to $5 \leq T \leq 2000$.

Figure 1 shows 38 curves of the specific heats, for $N = 6$, as functions of the temperature in the range $0.1 \leq T \leq 35$. Each curve is for a different integral value of c in the range $2, 3, \cdots, 39$. The central and dense part of the figure, where a large part of the curves have the same form, are those graphs that have a large c and, therefore, they may represent the solid crystals that are characterized by a periodic structure in which neighbouring occupied sites are widely separated. Indeed, these curves resemble, except for the sharp peaks, that of Debye which represents well the solid crystal. The other curves that differ from the central ones, and that generally have large values for the specific heats at small T, are those that have smaller c and, therefore, can not represent the solid crystal. These curves may represent some "soft" substance [11] in which the constituent atoms or molecules are closer to one another than in the solid crystal. These substances have Einstein frequencies [4,11] smaller than those of the solid crystals by a factor of 10 to 50 [11] and, therefore, are characterized by higher values of the specific heats. Also, the remarked sharp peaks have no derivative and this suggests an existence of phase transitions. Figure 2 shows 39 different curves of the specific heats, for $n = 35$, as functions of the temperature in the range $0.1 \leq T \leq 100$. Each curve is for a different integral value of c in the range $2, 3, \cdots, 40$. As in figure 1 the similar Debye like curves in the central part of the figure are for large c's and they may represent solid crystals, whereas the other curves are for small c's and they may represent, as in the former figure, "soft" substances. We note that seven of the curves have each a part below the Debye curves and a part above them and so they demonstrate the double peak phenomena found in antiferromagnetic [6] and superconducting materials [7]. The second peak, in our case, is obtained at a comparatively large value of the temperature ($T \approx 40$) compared to the values ($T \approx 1$) in [5–7]. Note also that the maximum values obtained by the curves of this figure are unity, whereas, most of the curves in the former figure have maxima that exceed unity. All the curves of figure 2 show, as in the former figure, for small values of T, peaks that are suggestive of phase transitions.

We can find the corresponding critical exponent [9] χ associated with these phase transitions by noting that we can write, in the neighbourhoud of the critical temperature T_c at which the specific heat has a phase transition, an analytical approximate expression for the specific heat as follows [9]

$$C_h(\epsilon) = A + B\epsilon^{\frac{1}{2}}, \tag{17}$$

where $\epsilon = \frac{T - T_c}{T_c}$. As seen, the first order derivative of this specific heat with respect to the temperature diverges at the point $T = T_c$ and so, the critical exponent χ is obtained as [9]

$$\chi = 1 + \lim_{\epsilon \to 0} \frac{ln|\grave{C}_h(\epsilon)|}{ln(\epsilon)} = 1 + \lim_{\epsilon \to 0} \frac{ln|\frac{B}{\epsilon^{\frac{1}{2}}}|}{ln|\epsilon|} = \frac{1}{2}, \tag{18}$$

where $\grave{C}_h(\epsilon)$ is the derivative of C_h from Eq (17) with respect to ϵ and the unity value of the first term denotes the order (which is 1 here) of the derivative of C_h from Eq (17) which diverges at $T = T_c$, that is, the appropriate critical exponent is $\frac{1}{2}$.

The conspicuous departure of the curve of the specific heat, for small c, from that of Debye can be explained by noting that the total number of nondegenerate energies that satisfies Eq (10) varies for different values of these c's. Moreover, we find, numerically, for all finite N and for small c, no energy from the lower part of the spectrum that satisfies Eq (10) for the $e < v$ case. That is, solutions of Eq (10) for this case are found, for small c's, only from the part of the spectrum that is close to the value of v. Thus, when we sum upon all the allowed energies, in order to calculate the average energy and the specific heat, the summation does not include the lower part of the spectrum. For example, the number of nondegenate allowed (energies) solutions of Eq (10), for $N = 6$, $e < v$ and $c = 1.5$ are only 3, whereas they amount to 311 for $c = 15$. That is, for the larger values of c we have a larger number of additional (that may be thousands for large potential v) allowed energies, and this yields entirely different values for the average energy $< e >$ and the specific heat C_h derived from it. Now, the large values of c correspond, as we have remarked, to the solid state crystals in which the interval between any two close atoms is large compared to the extent of such an atom, and the small values of c to the "soft" substances.

The entropy S and the specific heat C_h are related by [4] $C_h = T\frac{\partial S}{\partial T}$. Thus, from the last discussion we infer that also the change of the entropy S with the temperature T jumps at the same values of T in which the specific heat C_h jumps. That is, the change of the entropy with T has also phase transition. Moreover, the entropy S and the free energy F are related by the equation [4] $S = -\frac{\partial F}{\partial T}$, so that, differentiating both sides of the last relation with respect to the temperature T and using the relation between the specific heat C_h and the entropy S we obtain

$$C_h = T\frac{\partial S}{\partial T} = -T\frac{\partial^2 F}{\partial T^2} \tag{19}$$

From the last equation we see that the second derivative of the free energy F with respect to the temperature T also changes steeply at the same values of T in which C_h does so.

When c becomes very large we have $b >> a$, so that we may ignore a compared to b. Thus, writing the trigonometric functions of the components of T from Eq (4) as exponentials, substituting in Eq (6), and ignoring, as noted, a with respect to b we can see that the matrix Q from Eq (6) becomes in the limit of a very large c the two dimensional unit matrix. In this case Eq (10), from which the energy spectrum is obtained, becomes the same as Eq (12) from which the energy spectrum has been obtained as $e = k^2 = (\frac{\pi N}{C})^2$. But we note that whereas Eq (12) was obtained for the case of high energies only for which the index n begins from a large value n_0 ($n_0 = 941$), here, in the limit of very large c, n assumes all integer values of $n = 0, 1, 2, \ldots$. In this case the average energy is

$$< e >_{C_{h\to\infty}} (\beta) = \frac{\sum_{n=0}^{n=\infty} (\frac{\pi n}{C})^2 e^{-\beta(\frac{\pi n}{C})^2}}{\sum_{n=0}^{n=\infty} e^{-\beta(\frac{\pi n}{C})^2}} \tag{20}$$

Note that the average energy from the last equation does not depend upon the number of barriers N. The specific heat is

$$C_{h_{c\to\infty}} = \frac{\partial < e >_{C_{h\to\infty}}(\beta)}{\partial T} = \frac{1}{T^2}\left(\frac{\sum_0^\infty (\frac{\pi n}{C})^4 e^{-\beta(\frac{\pi n}{C})^2}}{\sum_0^\infty e^{-\beta(\frac{\pi n}{C})^2}} - \frac{\sum_{n=0}^{n=\infty}(\frac{\pi n}{C})^2 e^{-\beta(\frac{\pi n}{C})^2}\sum_{\grave{n}=0}^{\grave{n}=\infty}(\frac{\pi \grave{n}}{C})^2 e^{-\beta(\frac{\pi \grave{n}}{C})^2}}{\sum_{n=0}^{n=\infty} e^{-\beta(\frac{\pi n}{C})^2}\sum_{\grave{n}=0}^{\grave{n}=\infty} e^{-\beta(\frac{\pi \grave{n}}{C})^2}}\right) \tag{21}$$

Plotting the curve of the specific heat from the last equation as a function of the temperature (not shown here) one can see that at small T $C_{h_{\to\infty}}$ varies rapidly from zero to 0.52 from which it descends sharply to its asymptotic value of 0.5. The curve is not differentiable at the point at which it assumes the value of 0.52 and so this point appears to be a phase transition one.

III. THE ONE-DIMENSIONAL N POTENTIAL BARRIER SYSTEM FOR $N \to \infty$

We discuss, now, the case where the number of traps N tends to the limit $N \to \infty$. We may use for this case all the equations (1)-(6) derived for the finite N case in the previous section, so that taking the limit of a very large N one obtains from Eq (6) for the right hand side of the potential barrier system at the point $x = \frac{a+b}{2}$ where $n = N$

$$\begin{bmatrix} A_{2N+1} \\ B_{2N+1} \end{bmatrix} = \begin{bmatrix} e^{-ik(a+b)} & 0 \\ 0 & e^{ik(a+b)} \end{bmatrix} \left(\begin{bmatrix} e^{\frac{ikb}{N}} & 0 \\ 0 & e^{-\frac{ikb}{N}} \end{bmatrix} \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \right)^N \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} \tag{22}$$

The expression under the exponent N can be written, using the set (4), in the limit of very large N, as

$$\begin{aligned} &\left(\begin{bmatrix} e^{\frac{ikb}{N}} & 0 \\ 0 & e^{-\frac{ikb}{N}} \end{bmatrix} \begin{bmatrix} \cos(\frac{aq}{N}) + i\frac{\xi}{2}\sin(\frac{aq}{N}) & i\frac{\eta}{2}\sin(\frac{aq}{N}) \\ -i\frac{\eta}{2}\sin(\frac{aq}{N}) & \cos(\frac{aq}{N}) - i\frac{\xi}{2}\sin(\frac{aq}{N}) \end{bmatrix} \right)^N = \\ &= \left(\begin{bmatrix} (1+\frac{ikb}{N})(1+\frac{i\xi}{2}(\frac{aq}{N})) & i(1+\frac{ikb}{N})\frac{\eta}{2}(\frac{aq}{N}) \\ -i(1-\frac{ikb}{N})\frac{\eta}{2}(\frac{aq}{N}) & (1-\frac{ikb}{N})(1-\frac{i\xi}{2}(\frac{aq}{N})) \end{bmatrix} \right)^N = \\ &= \left(1 + \frac{i}{N}\left(\begin{bmatrix} kb + aq\frac{\xi}{2} & aq\frac{\eta}{2} \\ -aq\frac{\eta}{2} & -(kb + aq\frac{\xi}{2}) \end{bmatrix} \right)\right)^N = (1 + \frac{i}{N}((kb + aq\frac{\xi}{2})\sigma_3 + iaq\frac{\eta}{2}\sigma_2))^N \end{aligned} \tag{23}$$

The last equation is obtained by expanding in a Taylor series the cosine and sine functions and keep only terms of the order $\frac{1}{N}$. σ_2, and σ_3 are the two dimensional Pauli matrices $\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. Using the relation $\lim_{n\to\infty}(1 + \frac{c}{n})^n = e^c$, where c is some constant we obtain from equations (22)-(23)

$$\begin{bmatrix} A_{2N+1} \\ B_{2N+1} \end{bmatrix} = \exp(-ik(a+b)\sigma_3)\exp(i((kb + \frac{aq\xi}{2})\sigma_3 + \frac{iaq\eta}{2}\sigma_2)) \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} \tag{24}$$

We denote the two expressions under the second exponent as

$$f = kb + aq\frac{\xi}{2}, \quad d = aq\frac{\eta}{2} \tag{25}$$

Now, making use of the relation

$$(f\sigma_3 + id\sigma_2)^2 = f^2 - d^2 = \phi^2, \tag{26}$$

we can expand the second exponent on the right hand side of Eq (24) in a Taylor series, so that after collecting corresponding terms we obtain

$$e^{i((kb+aq\frac{\xi}{2})\sigma_3 + iaq\frac{\eta}{2}\sigma_2)} = \cos(\sqrt{f^2-d^2}) + \frac{i(f\sigma_3 + id\sigma_2)}{\sqrt{f^2-d^2}}\sin(\sqrt{f^2-d^2}) \tag{27}$$

Substituting from equations (25),(26) into Eq (24), and defining $z = k(a+b)$, we obtain

$$\begin{bmatrix} A_{2N+1} \\ B_{2N+1} \end{bmatrix} = \begin{bmatrix} e^{-iz}(\cos\phi + if\frac{\sin(\phi)}{\phi}) & ie^{-iz}d\frac{\sin(\phi)}{\phi} \\ -e^{iz}d\frac{\sin(\phi)}{\phi} & e^{iz}(\cos\phi - if\frac{\sin(\phi)}{\phi}) \end{bmatrix} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} \tag{28}$$

The last equations are obtained for the $e > v$ case. Using Eqs (13), (14) for the $e < v$ case and going through steps equivalent to those of the $e > v$ case we obtain the following matrix equation equivalent to Eq (28).

$$\begin{bmatrix} A_{2N+1} \\ B_{2N+1} \end{bmatrix} = \begin{bmatrix} e^{-iz}(\cos\grave{\phi} + \frac{i\grave{f}\sin(\grave{\phi})}{\grave{\phi}}) & -ie^{-iz}\frac{\grave{d}\sin(\grave{\phi})}{\grave{\phi}} \\ ie^{iz}\frac{\grave{d}\sin(\grave{\phi})}{\grave{\phi}} & e^{iz}(\cos\grave{\phi} - i\frac{\grave{f}\sin(\grave{\phi})}{\grave{\phi}}) \end{bmatrix} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}, \tag{29}$$

where $\grave{f}$, $\grave{d}$ and $\grave{\phi}$ are given by

$$\grave{f} = kb - \frac{aq\eta}{2}, \quad \grave{d} = \frac{aq\xi}{2}, \quad \grave{\phi}^2 = (\grave{f}\sigma_3 - i\grave{d}\sigma_2)^2 = \grave{f}^2 - \grave{d}^2 \tag{30}$$

We can, now, find the energy epectrum of the dense system in an equivalent way to the finite N case of the previous section. We obtain, for both cases of $e > v$ and $e < v$, similar equations to Eqs (7)-(8), but now the two dimensional matrix Q are those on the right hand side of Eqs (28),(29), where their four components are given explicitly. Note that the four components of the two dimensional matrix Q for the finite N (see Eq (6)) can be obtained only numerically. Thus, using, for the $e > v$ case, the explicit expression of Q from Eq (28) we can write the analogous equation (for $N \to \infty$) to Eq (10) as

$$\det\begin{bmatrix} \frac{e^{2ikC}}{Q_{22}} - 1 & \frac{e^{2ikC}Q_{12}}{Q_{22}} \\ -\frac{e^{2ikC}Q_{21}}{Q_{22}} & \frac{e^{2ikC}}{Q_{22}} - 1 \end{bmatrix} = \frac{e^{4ikC}}{Q_{22}^2} - \frac{2e^{2ikC}}{Q_{22}} + 1 + \frac{Q_{12}Q_{21}e^{4ikC}}{Q_{22}^2} = \tag{31}$$

$$= \cos(4kC)(1 + \frac{d^2\sin^2(\phi)}{\phi^2}) + \cos(2z)(\cos^2(\phi) - \frac{f^2\sin^2(\phi)}{\phi^2}) + \frac{2f\sin(\phi)}{\phi}(\sin(2z)\cos(\phi) -$$

$$-\sin(2kC+z)) - 2\cos(2kC+z)\cos(\phi) + i(\sin(4kC)(1 + \frac{d^2\sin^2(\phi)}{\phi^2}) + \sin(2z)(\cos^2(\phi) -$$

$$-\frac{f^2\sin^2(\phi)}{\phi^2}) + \frac{2f\sin(\phi)}{\phi}(\cos(2kC+z) - \cos(2z)\cos(\phi)) - 2\sin(2kC+z)\cos(\phi)) = 0$$

For the $e < v$ case we use the explicit expression of Q from Eq (29), together with Eqs (30), to obtain a similar equation to Eq (31) from which the energy spectrum for the $e < v$ case may be obtained.

The energy spectrum is composed from those energies that satisfy the real and imaginary parts of the last equation for the $e > v$ case and the corresponding one for the $e < v$ case. Thus, we may obtain the average energy $< e >_{N\to\infty} (c)$ for each value of c. From these average energies we obtain the corresponding specific heats C_h as functions of c and T. The dependence of C_h upon the temperature T, as a function of c, is, for small T, different from the dependence discussed in the previous section for finite N. That is, C_h jumps up to its peaked value from which it immediately jumps down to rise again to anther higher maximum. We note that, generally, for finite N there is only one peaked maximum, and although in Figure 2 we see that several curves have double peaks, nevertheless, this is only for small c and that when c grows the curves become the same as that of Debye as seen in the dense central part of Figure 2 which are for large c. Compared to this the double peak appearance of the specific heat curves for infinite N is retained even for large c as can be seen from Figure 3 which is drawn for $c = 200$. Figure 4 shows 30 different curves of the specific heats as function of the temperature. Each curve is for a different value of c from $0.3, 0.4, \cdots, 3.2$. Note the large difference in the heights of the two peaks, and that both are points where the first derivative with respect to the temperature T does not exist and so they appear to be phase transition points. A similar discussion to that of the finite N case (see also Eqs (17), (18) yields a critical exponent of $\frac{1}{2}$ for both peaks. we infer that also the first derivative of the entropy S and the second derivative of the free energy F, both with respect to the temperature, change in a discontinuous way at the same values of T (see the analogous discussion at the previous section). When the temperature increases all the curves tend to the value of 0.55 as for the finite N case. When c becomes very large the curves (not shown here) of the specific heats become similar to each other and to the Debye graph.

IV. CONCLUDING REMARKS

We have shown that the one-dimensional multibarrier potential of finite range shows signs of phase transitions for certain values of the temperature T. These phase transitions depend upon the number of barriers N and the ratio c of the total spacing to their total width and are demonstrated for both cases of finite and infinite number N as shown in figures 1-4 and also for small and large values of c. Moreover, it is seen from the curves of the specific heat as a function of the temperature for $N = 35$ and small c (see Figure 2) and for infinite N and a large range of c (see Figures 3 and 4) that the phase transitions appear in a double peak form. Double peaks have been seen in antiferromagnetic and superconducting materials and are apparently associated with dynamically induced phase transitions [6,7], and in the quark-gluon plasma [8].

We note that we have found [1] that the one-dimensional multibarrier system discussed here demonstrates also, for large N, a unit value for the transmission probability and signs of chaos which may be interpreted in terms of effective decoherence and the space analog [14] of the Zeno effect [12] in which a very large number of repetitions of the same experiment (interaction), in a finite total time, preserves the initial state of the system. It has also been shown [13,14] that a beam of light that passes through a large number of analyzers arrayed along a finite interval of a spatial axis, a configuration which is very similar to the

one discussed here, remains after the passage with the same initial polarization and intensity it had before passing. This kind of preservation of the initial "state" by passing through a large number of physical apparatuses, each of them is supposed by itself to change the state of the passing system, has also been shown in the *classical* regime [15] where the initial density of classical particles passing through a one dimensional array of imperfect traps [16] remains at the same value it had before the passage if the ratio of the total spacing to width (which corresponds to the ratio c here) increases.

Thus, our finding here that when c grows the curves of the specific heat, as functions of the temperature T, become similar to the known graph of Debye [4], indicates that the system makes a transition to the physical situation which corresponds to a solid crystal.

We have found that the critical exponents associated with these phase transitions have the value $\frac{1}{2}$. The other statistical parameters associated with the specific heat such as the entropy and the free energy also demonstrate, in the rate of their changes with respect to the temperature T, the same type of behaviour at the same values of N, c, and T.

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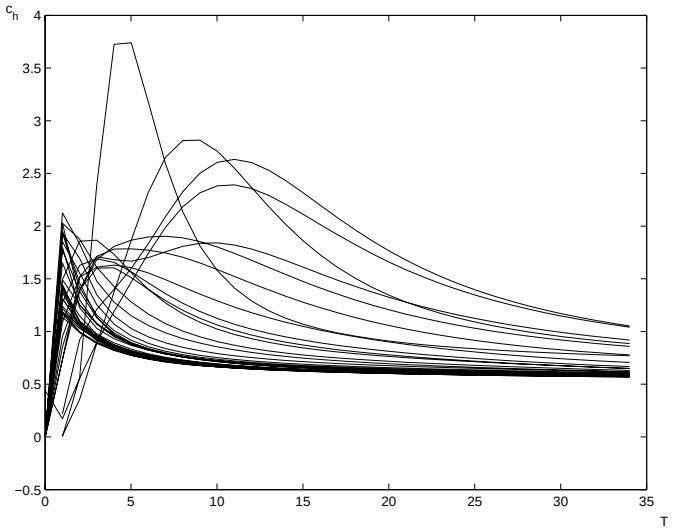

FIG. 1. 38 different curves of the specific heat as a function of the temperature for $N = 6$ and the following integral values of $c = 2, 3 \cdots 39$. The dense central part of the graph are the curves obtained for the larger values of c and they all resemble, except for the sharp peaks at the left, the Debye's graph for solid crystals. The curves are not differentiable at the sharp peaks and so they have phase transition at these points. The other curves are for small c and they represent the "soft" substances that have a comparable low Einstein frequencies and therefore a high values of the specific heats.

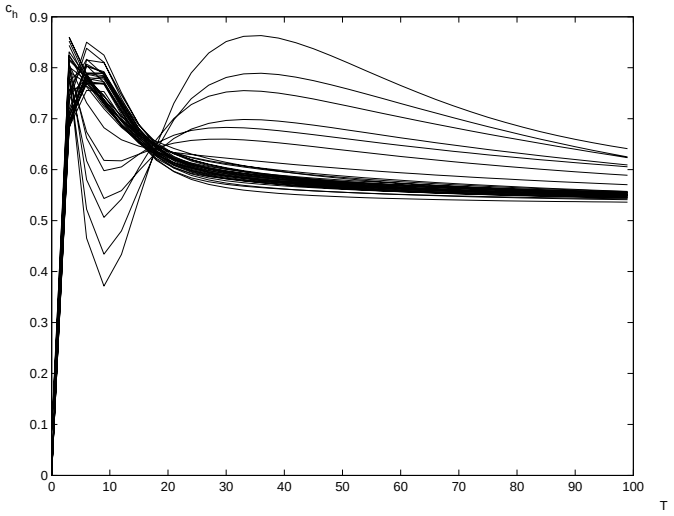

FIG. 2. 39 different curves of the specific heat as a function of the temperature for $n = 35$ and for the following integral values of $c = 2, 3 \cdots 40$. As in figure 1 the dense central part of the figure are the curves that represent the Debye curve, except for the sharp peaks at the left at which the specific heats are not differentiable and so are points of phase transition. Note that seven of the curves have a part below the dense section and a part above it.

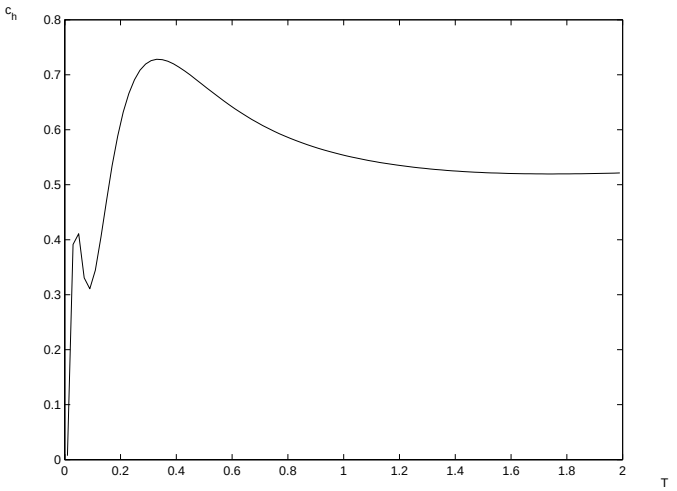

FIG. 3. Double peak of the specific heat as a function of the temperature for infinite N and for $c = 200$. Note the difference between the heights of the two maxima.

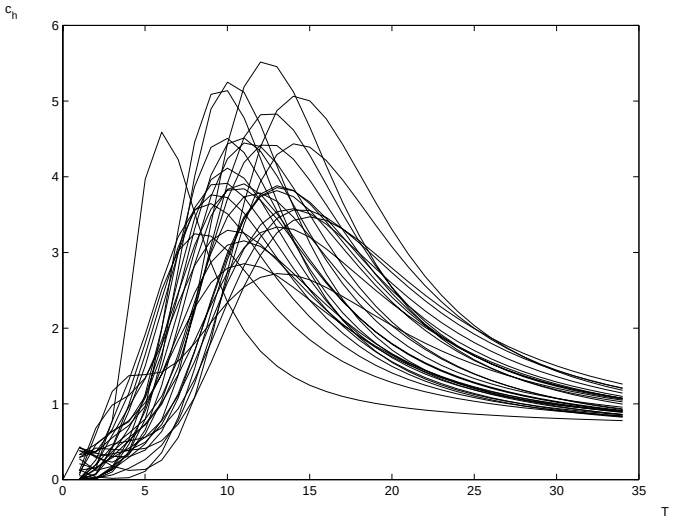

FIG. 4. 30 different curves of the specific heat as a function of the temperature for infinite N ans for the following values of $c = 0.3, 0.4, \cdots 3.2$. All the curves tend to the value of 0.55 for large T. Note that the second peak of each curve is much larger than the first and that all these second peaks are obtained for $T > 5$. The peaks of each curve are not differentiable and so they are suggestive of phase transitions.